Supporting Information for Conformational Analysis of 3-(Trimethylsilyl)-propionic Acid by NMR Spectroscopy: An Unusual Expression of the β-Silyl Effect

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General Experimental Methods

Materials

4,4-Dimethylpentanoic acid was synthesized by Françoise Gregoire.

Sample preparation

NMR samples of 3-(trimethylsilyl)-propionic acid in water, dimethyl sulfoxide, methanol, ethanol, isopropyl alcohol, *tert*-butyl alcohol, tetrahydrofuran, and toluene were prepared with constant concentrations of 0.05 M.

The acid was prepared by dissolving equivalents of sodium 3-(trimethylsilyl)-propionate and sodium bisulfate in water and ethanol.

To ensure completion of the reaction, the mixture was evaporated to dryness under reduced pressure to remove the water and ethanol. The resulting sodium sulfate was filtered after dissolution in the dissolved deuterated solvent. The anion was prepared by dissolving sodium 3-(trimethylsilyl)-propionate and 1.0 equiv. of tetrabutylammonium bromide in ethanol and evaporated to dryness under reduced pressure. The resulting mixture was taken up in each deuterated solvent and filtered from the residual sodium bromide.

Spectral acquisition

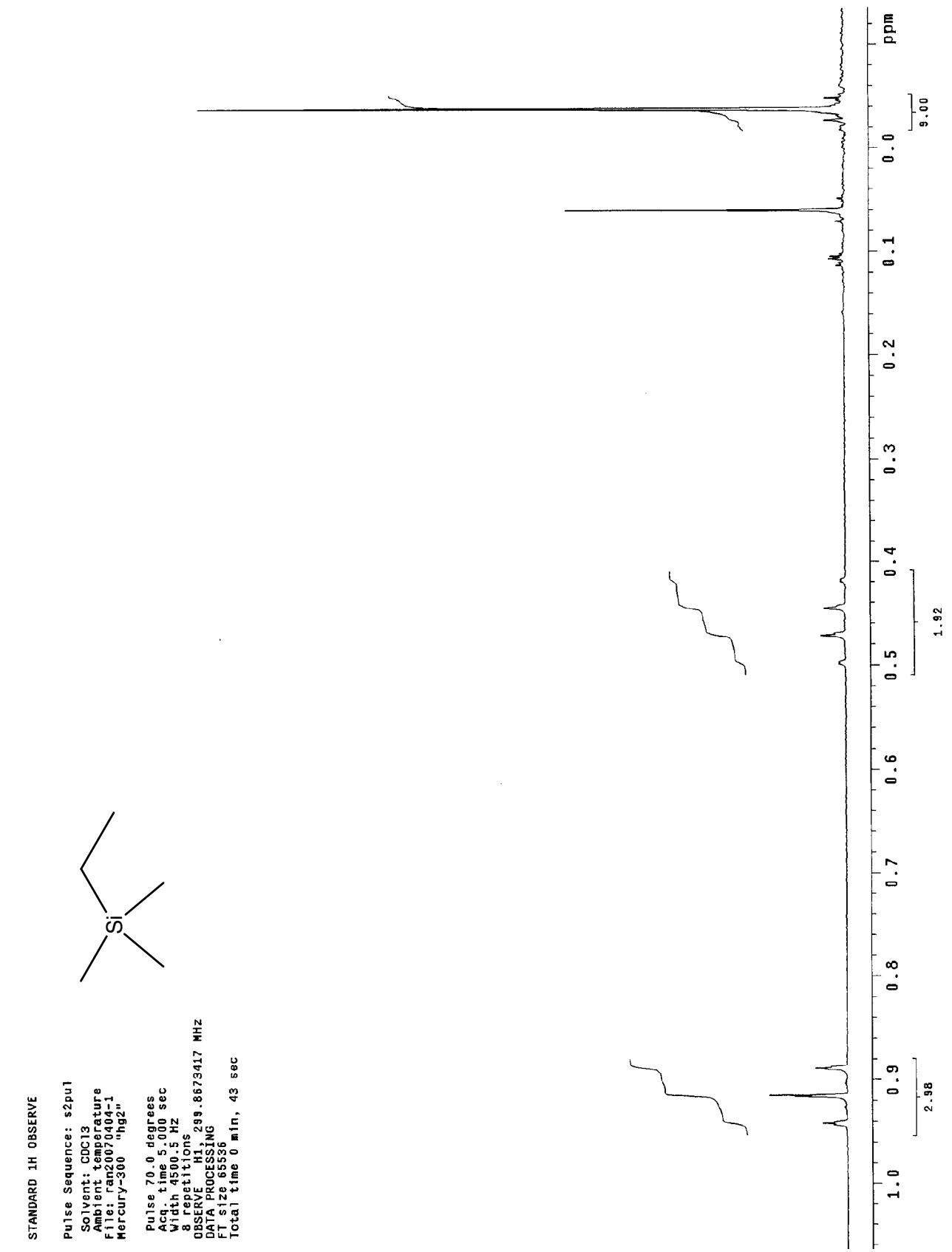
^{1}H NMR spectra were acquired for all solvent samples at ambient temperature with either a 300 MHz or 600 MHz NMR spectrometer with signal lock on the deuterated solvent. The ^{1}H NMR peaks were referenced to known chemical-shift positions of the alcohols and/or TMS.

Determination of λ for the trimethylsilyl, carboxyl, and carboxylate substituent

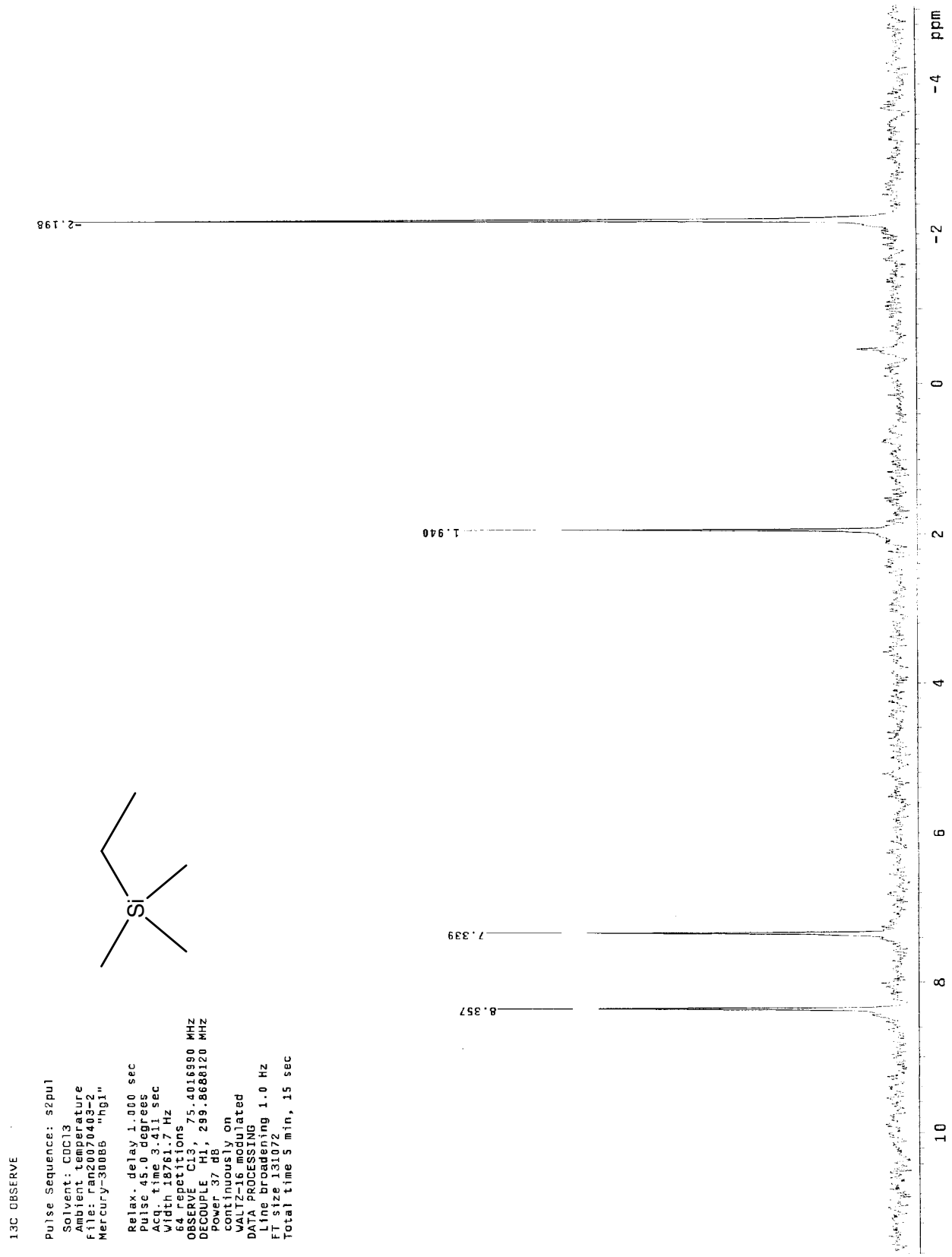
One drop of ethyltrimethylsilane was added to 0.75 mL each of the target solvents, water, dimethyl sulfoxide, methanol, isopropyl alcohol, and *tert*-butyl alcohol. The ^{1}H NMR spectra of each sample were taken on a 300 MHz spectrometer. The resulting A_2B_3 spectra were analyzed with gNMR to obtain the

vicinal coupling constant for use in determining λ for the trimethylsilyl substituent in the solvents of interest.[6] The λ value for the trimethylsilyl substituent in each target solvents was -0.37 indicating that the substituent was less electronegative than hydrogen with a reported λ value of -0.18.[6] The same procedure for propionic acid afforded a value for the carboxyl group independent of solvent of 0.39, which is the λ value reported by Altona.[6] For determination of λ for the carboxylate substituent, tetrabutylammonium propionate was prepared by mixing propionic acid with sodium hydroxide solution until the pH was neutral. One equiv. of tetrabutylammonium bromide dissolved in ethanol was then added and the mixture evaporated to dryness under reduced pressure to remove the ethanol. One drop of liquid was added to 0.75 ml of the deuterated solvents, water, dimethyl sulfoxide, methanol, *tert*-butyl alcohol, tetrahydrofuran, and toluene. The resulting mixture was filtered from the residual sodium bromide. The ^{1}H NMR spectra at 300 MHz for the ethyl vicinal coupling constant, converted to λ values for the carboxylate substituent, had more variation than for the unassociated acid being 0.44 in water, 0.43 in dimethyl sulfoxide, 0.35 in methanol, 0.35 in *tert*-butyl alcohol, 0.41 in tetrahydrofuran, and 0.27 in toluene. The λ value of 0.29 for the carboxylate group in water is reported by Altona.[6] A λ value for the sulfonate group is reported by Gregoire[11] of 0.59, from measurements on sodium ethanesulfonate in D_2O.

^{1}H NMR of Ethyltrimethylsilane



^{13}C NMR of Ethyltrimethylsilane



Gauche 3-(trimethylsilyl)-propionic acid

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                *             FROM IOWA STATE UNIVERSITY          *
                * M.W.SCHMIDT, K.K.BALDRIDGE, J.A.BOATZ, S.T.ELBERT, *
                *   M.S.GORDON, J.H.JENSEN, S.KOSEKI, N.MATSUNAGA,   *
                *          K.A.NGUYEN, S.J.SU, T.L.WINDUS,          *
                *       TOGETHER WITH M.DUPUIS, J.A.MONTGOMERY      *
                *         J.COMPUT.CHEM.  14, 1347-1363(1993)       *
                ****************** PC-UNIX VERSION *****************

SINCE 1993, STUDENTS AND POSTDOCS WORKING AT IOWA STATE UNIVERSITY
AND ALSO IN THEIR VARIOUS JOBS AFTER LEAVING ISU HAVE MADE IMPORTANT
CONTRIBUTIONS TO THE CODE:
IVANA ADAMOVIC, CHRISTINE AIKENS, YURI ALEXEEV, POOJA ARORA, ROB BELL,
PRADIPTA BANDYOPADHYAY, JONATHAN BENTZ, BRETT BODE, GALINA CHABAN,
WEI CHEN, CHEOL HO CHOI, PAUL DAY, TIM DUDLEY, DMITRI FEDOROV,
GRAHAM FLETCHER, MARK FREITAG, KURT GLAESEMANN, GRANT MERRILL,
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MIKE PAK, JIM SHOEMAKER, LYUDMILA SLIPCHENKO, JIE SONG,
TETSUYA TAKETSUGU, SIMON WEBB.

ADDITIONAL CODE HAS BEEN PROVIDED BY COLLABORATORS IN OTHER GROUPS:
IOWA STATE UNIVERSITY: JOE IVANIC, KLAUS RUEDENBERG
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NAKAJIMA, TAKAO TSUNEDA, MUNEAKI KAMIYA, SUSUMU YANAGISAWA,
KIYOSHI YAGI, MAHITO CHIBA
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NATIONAL INST. OF STANDARDS AND TECHNOLOGY: WALT STEVENS, DAVID GARMER
UNIVERSITY OF PISA: BENEDETTA MENNUCCI, JACOPO TOMASI
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FENG LONG GU, JACEK KORCHOWIEC, MARCIN MAKOWSKI, AND YURIKO AOKI
PENNSYLVANIA STATE UNIVERSITY:
TZVETELIN IORDANOV, CHET SWALINA, SHARON HAMMES-SCHIFFER

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6 C	6.678602	-0.678602	6.659463	-0.659463
7 H	0.832029	0.167971	0.807480	0.192520
8 H	0.850420	0.149580	0.816013	0.183987
9 C	5.883410	0.116590	5.795698	0.204302
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5	15	1.096	0.965	6	16	1.096	0.965	6	17	1.096	0.967
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5 C	3.726	3.726	0.000
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Gauche 3-(trimethylsilyl)-propionate

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INPUT CARD> H           1.0   0.9445954043   0.2737663180   2.9039107503
INPUT CARD> H           1.0  -2.4948422660   0.8999668004   0.1788863271
INPUT CARD> H           1.0  -3.1233541202  -0.6952974132  -0.1996061144
INPUT CARD> O           8.0  -2.7930057805   0.2491293568  -2.5521721794
INPUT CARD> O           8.0  -0.6025628702   0.2984196972  -1.9464718467
INPUT CARD> $END
62000000 WORDS OF MEMORY AVAILABLE


NSERCH= 17     ENERGY=    -676.2602342

-----------------------
GRADIENT (HARTREE/BOHR)
-----------------------
ATOM           ZNUC       DE/DX         DE/DY         DE/DZ
------------------------------------------------------------
1  C            6.0     0.0000138    -0.0000531    -0.0000164
2  C            6.0     0.0000183     0.0000288     0.0000596
3  SI          14.0    -0.0000093     0.0000282    -0.0000324
4  C            6.0     0.0000201    -0.0000052     0.0000124
5  C            6.0    -0.0000176    -0.0000124     0.0000226
6  C            6.0     0.0000024    -0.0000392     0.0000067
7  H            1.0     0.0000031     0.0000352     0.0000164
8  H            1.0    -0.0000004    -0.0000044    -0.0000028
9  C            6.0     0.0000312     0.0000193    -0.0000867
10  H           1.0    -0.0000167     0.0000025    -0.0000105
11  H           1.0    -0.0000040    -0.0000058     0.0000064
12  H           1.0    -0.0000082    -0.0000173    -0.0000198
13  H           1.0     0.0000025     0.0000088     0.0000018
14  H           1.0    -0.0000057     0.0000087    -0.0000067
15  H           1.0    -0.0000009     0.0000041    -0.0000004
16  H           1.0     0.0000022     0.0000103     0.0000055
17  H           1.0    -0.0000021     0.0000098    -0.0000098
18  H           1.0     0.0000063     0.0000053     0.0000147
19  H           1.0    -0.0000065     0.0000063    -0.0000010
20  H           1.0    -0.0000117    -0.0000174     0.0000036
21  O           8.0     0.0000333    -0.0000039     0.0000090
22  O           8.0    -0.0000502    -0.0000090     0.0000279
```

MAXIMUM GRADIENT = 0.0000867 RMS GRADIENT = 0.0000216

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-1.0545360194	-0.7147204443	0.5586255426
C	6.0	-2.1988897741	-0.0617545402	-0.2361447163
SI	14.0	0.6838471917	0.0685129863	0.3921707090
C	6.0	0.6722019149	1.9613239854	0.2293595709
C	6.0	1.8949294304	-0.7746461288	-0.8053404446
C	6.0	1.4781288442	-0.2512209279	2.1315653313
H	1.0	-0.9529455030	-1.7686693782	0.2549680586
H	1.0	-1.2988602873	-0.7319243277	1.6323934336
C	6.0	-1.8728582711	0.1868745359	-1.7383606521
H	1.0	0.0487017391	2.4109769928	1.0144614111
H	1.0	0.2647256394	2.2426415166	-0.7447969242
H	1.0	1.6834604290	2.3794735755	0.3326741351
H	1.0	2.9250371902	-0.4359396647	-0.6285407142
H	1.0	1.6001580654	-0.5597208451	-1.8349301083
H	1.0	1.8770995998	-1.8633372566	-0.6583829306
H	1.0	2.5245792966	0.0811179331	2.1640599152
H	1.0	1.4607936423	-1.3205009650	2.3860556671
H	1.0	0.9311364782	0.2849648235	2.9190833677
H	1.0	-2.4422508920	0.9205424033	0.1981002905
H	1.0	-3.1213481078	-0.6537316482	-0.1749517505
O	8.0	-2.8467451366	0.3202187367	-2.5181626120
O	8.0	-0.6333724700	0.2619086374	-2.0053365800

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1 C	6.579904	-0.579904	6.511350	-0.511350
2 C	6.281293	-0.281293	6.329460	-0.329460
3 SI	12.744181	1.255819	13.413300	0.586700
4 C	6.798760	-0.798760	6.669359	-0.669359
5 C	6.791380	-0.791380	6.660076	-0.660076
6 C	6.739435	-0.739435	6.713045	-0.713045
7 H	0.867142	0.132858	0.820779	0.179221
8 H	0.886561	0.113439	0.836498	0.163502
9 C	5.646072	0.353928	5.844638	0.155362
10 H	0.870565	0.129435	0.828484	0.171516
11 H	0.795440	0.204560	0.796096	0.203904
12 H	0.877710	0.122290	0.835987	0.164013
13 H	0.882350	0.117650	0.839802	0.160198
14 H	0.786195	0.213805	0.794844	0.205156
15 H	0.875000	0.125000	0.833388	0.166612
16 H	0.871523	0.128477	0.838293	0.161707
17 H	0.867802	0.132198	0.836121	0.163879
18 H	0.869585	0.130415	0.834098	0.165902
19 H	0.874484	0.125516	0.826481	0.173519
20 H	0.873402	0.126598	0.832276	0.167724
21 O	8.616893	-0.616893	8.524464	-0.524464
22 O	8.604322	-0.604322	8.581163	-0.581163

BOND ORDER AND VALENCE ANALYSIS BOND ORDER THRESHOLD=0.050

ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER
1	2	1.539	0.884	1	3	1.914	0.813	1	7	1.102	0.967
1	8	1.101	0.976	1	19	2.175	-0.053	2	9	1.557	0.942
2	19	1.101	0.971	2	20	1.098	0.939	2	21	2.403	-0.076
2	22	2.384	-0.115	3	4	1.900	0.776	3	5	1.900	0.770
3	6	1.939	0.680	3	11	2.489	-0.062	3	14	2.489	-0.074
3	22	2.742	0.173	4	10	1.099	0.974	4	11	1.093	0.994
4	12	1.099	0.977	4	22	3.096	-0.075	5	13	1.099	0.978
5	14	1.092	1.003	5	15	1.099	0.973	6	16	1.098	0.984
6	17	1.099	0.987	6	18	1.099	0.985	9	21	1.255	1.675

```
9     22  1.270  1.512

                     TOTAL        BONDED         FREE
ATOM                VALENCE      VALENCE      VALENCE
1 C                  3.595        3.595        0.000
2 C                  3.437        3.437        0.000
3 SI                 2.962        2.962        0.000
4 C                  3.664        3.664        0.000
5 C                  3.714        3.714        0.000
6 C                  3.567        3.567        0.000
7 H                  0.949        0.949        0.000
8 H                  0.949        0.949        0.000
9 C                  4.179        4.179        0.000
10 H                 0.953        0.953        0.000
11 H                 0.939        0.939        0.000
12 H                 0.954        0.954        0.000
13 H                 0.953        0.953        0.000
14 H                 0.933        0.933        0.000
15 H                 0.955        0.955        0.000
16 H                 0.954        0.954        0.000
17 H                 0.952        0.952        0.000
18 H                 0.954        0.954        0.000
19 H                 0.945        0.945        0.000
20 H                 0.946        0.946        0.000
21 O                 1.565        1.565        0.000
22 O                 1.456        1.456        0.000

---------------------
ELECTROSTATIC MOMENTS
---------------------

POINT   1           X           Y           Z (BOHR)    CHARGE
-0.572658    0.213266   -0.687678       -1.00 (A.U.)
DX          DY          DZ          /D/  (DEBYE)
4.390696   -0.730794    6.630216    7.985739
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =     3.30 TOTAL CPU TIME =    24618.2 (  410.3 MIN)
TOTAL WALL CLOCK TIME=    66531.9 SECONDS, CPU UTILIZATION IS  37.00%
$VIB
IVIB=   0 IATOM=   0 ICOORD=   0 E=     -676.2602342253
1.375914245E-05-5.306024985E-05-1.643297937E-05 1.834592379E-05 2.879748739E-05
5.961095136E-05-9.287327224E-06 2.818648655E-05-3.241630501E-05 2.014969329E-05
-5.214209998E-06 1.240814713E-05-1.759532718E-05-1.235197534E-05 2.256748210E-05
2.423961113E-06-3.920516436E-05 6.683342536E-06 3.053932590E-06 3.517405031E-05
1.638530026E-05-4.036515437E-07-4.370567891E-06-2.809152544E-06 3.121687846E-05
1.933770494E-05-8.666444381E-05-1.670456609E-05 2.527828338E-06-1.052281171E-05
-3.981157161E-06-5.777614527E-06 6.431473075E-06-8.184185226E-06-1.725104076E-05
-1.981893207E-05 2.491628408E-06 8.821062348E-06 1.765338920E-06-5.711000281E-06
8.727316806E-06-6.719931933E-06-9.380822923E-07 4.146478724E-06-3.742723239E-07
2.159425397E-06 1.029783946E-05 5.539223157E-06-2.051490643E-06 9.763449510E-06
-9.813839434E-06 6.339333076E-06 5.317670194E-06 1.472352602E-05-6.469254107E-06
6.339326314E-06-1.017032999E-06-1.169339675E-05-1.736598325E-05 3.591623739E-06
3.327744852E-05-3.876461390E-06 9.014008324E-06-5.019792859E-05-8.963433510E-06
2.786928458E-05
4.390695793E+00-7.307937347E-01 6.630216096E+00
......END OF GEOMETRY SEARCH......
STEP CPU TIME =     0.17 TOTAL CPU TIME =    24618.3 (  410.3 MIN)
TOTAL WALL CLOCK TIME=    66532.1 SECONDS, CPU UTILIZATION IS  37.00%
1326317  WORDS OF DYNAMIC MEMORY USED
EXECUTION OF GAMESS TERMINATED NORMALLY Fri Mar 30 05:46:12 2007
DDI: 262808 bytes (0.3 MB / 0 MWords) used by master data server.
```

Trans 3-(trimethylsilyl)-propionic acid

```
ECHO OF THE FIRST FEW INPUT CARDS -
INPUT CARD> $CONTRL RUNTYP=OPTIMIZE $END
INPUT CARD> $DFT DFTTYP=B3LYP $END
INPUT CARD> $BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.T. $END
INPUT CARD> $SYSTEM BALTYP=LOOP $END
INPUT CARD> $SYSTEM TIMLIM=600 MWORDS=18.75 $END
INPUT CARD>
INPUT CARD> $DATA
INPUT CARD>untitled
INPUT CARD>C1
INPUT CARD> C           6.0  -0.6665763545  -0.5257252793   0.4970932766
INPUT CARD> C           6.0  -1.6403086538  -0.2720148039  -0.6575964786
INPUT CARD> C           6.0  -2.9788511416  -0.9648360840  -0.4908340323
INPUT CARD> SI         14.0   1.0608753153   0.2564055550   0.3116280283
INPUT CARD> C           6.0   0.9186883169   2.1476976318   0.2432329673
INPUT CARD> C           6.0   1.8990086714  -0.3793422677  -1.2684771097
INPUT CARD> C           6.0   2.0867583274  -0.2284857950   1.8315472607
INPUT CARD> O           8.0  -3.3264000878  -1.6497095061   0.4478784706
INPUT CARD> O           8.0  -3.7959391910  -0.7296273633  -1.5541666115
INPUT CARD> H           1.0  -0.5450259551  -1.6083521421   0.6332067901
INPUT CARD> H           1.0  -1.1146009326  -0.1675190389   1.4336965435
INPUT CARD> H           1.0  -1.2285431435  -0.6032663882  -1.6200583257
INPUT CARD> H           1.0  -1.8527236705   0.7971434600  -0.7879390500
INPUT CARD> H           1.0   0.4937307935   2.5384884099   1.1758355666
INPUT CARD> H           1.0   0.2823715847   2.4855697685  -0.5826919422
INPUT CARD> H           1.0   1.9034478263   2.6120311719   0.1107365200
INPUT CARD> H           1.0   2.9393307553  -0.0390588512  -1.3207683391
INPUT CARD> H           1.0   1.3887062884  -0.0250362422  -2.1717727364
INPUT CARD> H           1.0   1.9080694336  -1.4757647417  -1.2964288507
INPUT CARD> H           1.0   3.0560415884   0.2848364649   1.8282509688
INPUT CARD> H           1.0   2.2784536016  -1.3067089558   1.8665265405
INPUT CARD> H           1.0   1.5637960706   0.0522098297   2.7526433060
INPUT CARD> H           1.0  -4.6303114430  -1.1989368324  -1.3815437632
INPUT CARD> $END
18000000 WORDS OF MEMORY AVAILABLE


NSERCH=  9     ENERGY=    -676.8152574

------------------------
GRADIENT (HARTREE/BOHR)
------------------------
ATOM             ZNUC       DE/DX         DE/DY         DE/DZ
-------------------------------------------------------------
1  C            6.0     0.0000307    -0.0000352    -0.0000308
2  C            6.0    -0.0000304     0.0000509     0.0000549
3  C            6.0    -0.0000645     0.0000176    -0.0000378
4  SI          14.0     0.0000180     0.0000241     0.0000042
5  C            6.0     0.0000077     0.0000082    -0.0000166
6  C            6.0    -0.0000058    -0.0000277    -0.0000097
7  C            6.0     0.0000015    -0.0000259     0.0000159
8  O            8.0     0.0000280    -0.0000300     0.0000846
9  O            8.0     0.0000155     0.0000442    -0.0000888
10  H           1.0     0.0000463    -0.0000382     0.0000297
11  H           1.0    -0.0000403     0.0000021    -0.0000218
12  H           1.0    -0.0000289    -0.0000206    -0.0000079
13  H           1.0     0.0000235    -0.0000083     0.0000033
14  H           1.0    -0.0000029     0.0000026     0.0000082
15  H           1.0    -0.0000204     0.0000076     0.0000022
16  H           1.0    -0.0000008     0.0000011     0.0000039
17  H           1.0     0.0000123     0.0000114    -0.0000086
18  H           1.0     0.0000088     0.0000049    -0.0000018
19  H           1.0    -0.0000056    -0.0000019     0.0000016
20  H           1.0     0.0000102     0.0000025     0.0000086
21  H           1.0    -0.0000020     0.0000136    -0.0000022
22  H           1.0    -0.0000012     0.0000066    -0.0000033
23  H           1.0     0.0000002    -0.0000096     0.0000120
```

```
MAXIMUM GRADIENT =  0.0000888    RMS GRADIENT = 0.0000263

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF ALL ATOMS ARE (ANGS)
ATOM        CHARGE       X              Y              Z
------------------------------------------------------------
C            6.0  -0.6670861608  -0.5225548966   0.4972913142
C            6.0  -1.6424152581  -0.2692089418  -0.6564582249
C            6.0  -2.9752445400  -0.9742517248  -0.4960533013
SI          14.0   1.0617348600   0.2578792675   0.3107804551
C            6.0   0.9225645529   2.1496740546   0.2410420686
C            6.0   1.8987397199  -0.3835481541  -1.2680338245
C            6.0   2.0845034252  -0.2261943958   1.8332211236
O            8.0  -3.3068819178  -1.6924856190   0.4231685896
O            8.0  -3.8061474425  -0.7097715480  -1.5415042649
H            1.0  -0.5457361537  -1.6052593747   0.6349942689
H            1.0  -1.1137301447  -0.1624356219   1.4339071963
H            1.0  -1.2282505963  -0.5938071983  -1.6202552335
H            1.0  -1.8622290413   0.7987548497  -0.7822421633
H            1.0   0.4994804363   2.5404510451   1.1746636187
H            1.0   0.2847491793   2.4893533467  -0.5830854369
H            1.0   1.9076289410   2.6130148775   0.1072711657
H            1.0   2.9388766210  -0.0427941955  -1.3238482608
H            1.0   1.3868410626  -0.0329845827  -2.1718535197
H            1.0   1.9080190293  -1.4800687754  -1.2913480534
H            1.0   3.0560654158   0.2829908474   1.8300117821
H            1.0   2.2713057947  -1.3049397464   1.8722710290
H            1.0   1.5614379906   0.0604497325   2.7524887622
H            1.0  -4.6342277736  -1.1922652460  -1.3764300913


TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS
ATOM            MULL.POP.    CHARGE          LOW.POP.     CHARGE
1 C              6.675991   -0.675991         6.496461   -0.496461
2 C              6.245989   -0.245989         6.288033   -0.288033
3 C              5.610697    0.389303         5.775173    0.224827
4 SI            12.932539    1.067461        13.438592    0.561408
5 C              6.697085   -0.697085         6.667384   -0.667384
6 C              6.705664   -0.705664         6.659690   -0.659690
7 C              6.666106   -0.666106         6.659009   -0.659009
8 O              8.465495   -0.465495         8.353466   -0.353466
9 O              8.457475   -0.457475         8.366464   -0.366464
10 H             0.836961    0.163039         0.806880    0.193120
11 H             0.839935    0.160065         0.807022    0.192978
12 H             0.825810    0.174190         0.802160    0.197840
13 H             0.825578    0.174422         0.804214    0.195786
14 H             0.842667    0.157333         0.819688    0.180312
15 H             0.844425    0.155575         0.820758    0.179242
16 H             0.840950    0.159050         0.821698    0.178302
17 H             0.840472    0.159528         0.821946    0.178054
18 H             0.843472    0.156528         0.820530    0.179470
19 H             0.842069    0.157931         0.821875    0.178125
20 H             0.843334    0.156666         0.822070    0.177930
21 H             0.842744    0.157256         0.822535    0.177465
22 H             0.842947    0.157053         0.819784    0.180216
23 H             0.631596    0.368404         0.684566    0.315434

--------------------------------
BOND ORDER AND VALENCE ANALYSIS     BOND ORDER THRESHOLD=0.050
--------------------------------

                  BOND                          BOND                          BOND
ATOM  PAIR DIST   ORDER      ATOM PAIR DIST     ORDER      ATOM PAIR DIST     ORDER
1      2  1.532  0.859        1   3  2.553  0.050          1   4  1.906  0.818
1      8  2.888  0.121        1  10  1.098  0.942          1  11  1.098  0.941
2      3  1.516  1.048        2   8  2.442 -0.172          2  12  1.098  0.925
2     13  1.098  0.922        3   8  1.213  1.906          3   9  1.361  0.926
4      5  1.898  0.872        4   6  1.899  0.879          4   7  1.897  0.821
5     14  1.097  0.965        5  15  1.096  0.969          5  16  1.097  0.965
6     17  1.096  0.965        6  18  1.096  0.968          6  19  1.097  0.966
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7     20  1.097  0.963        7  21  1.095  0.966        7  22  1.096  0.964
9     23  0.973  0.795

                     TOTAL       BONDED        FREE
ATOM                VALENCE     VALENCE     VALENCE
1 C                  3.694       3.694       0.000
2 C                  3.530       3.530       0.000
3 C                  4.044       4.044       0.000
4 SI                 3.292       3.292       0.000
5 C                  3.701       3.701       0.000
6 C                  3.713       3.713       0.000
7 C                  3.663       3.663       0.000
8 O                  1.875       1.875       0.000
9 O                  1.726       1.726       0.000
10 H                 0.944       0.944       0.000
11 H                 0.944       0.944       0.000
12 H                 0.937       0.937       0.000
13 H                 0.937       0.937       0.000
14 H                 0.948       0.948       0.000
15 H                 0.949       0.949       0.000
16 H                 0.948       0.948       0.000
17 H                 0.948       0.948       0.000
18 H                 0.948       0.948       0.000
19 H                 0.947       0.947       0.000
20 H                 0.949       0.949       0.000
21 H                 0.949       0.949       0.000
22 H                 0.949       0.949       0.000
23 H                 0.859       0.859       0.000

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ELECTROSTATIC MOMENTS
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POINT   1           X           Y           Z (BOHR)    CHARGE
-1.062544   -0.407932   -0.086923         0.00 (A.U.)
DX          DY          DZ          /D/  (DEBYE)
0.775976    0.977148   -1.059299    1.636787
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =     3.41 TOTAL CPU TIME =    13018.0 (  217.0 MIN)
TOTAL WALL CLOCK TIME=    19128.4 SECONDS, CPU UTILIZATION IS  68.06%
$VIB
IVIB=   0 IATOM=   0 ICOORD=   0 E=     -676.8152573769
3.069149146E-05-3.521620943E-05-3.084894448E-05-3.042575446E-05 5.090837482E-05
5.493587020E-05-6.446867603E-05 1.755000750E-05-3.779735213E-05 1.803094130E-05
2.411768322E-05 4.237767029E-06 7.705463113E-06 8.249482458E-06-1.656726527E-05
-5.794191241E-06-2.765210331E-05-9.663148821E-06 1.532165524E-06-2.586795406E-05
1.585815174E-05 2.795278597E-05-3.000260450E-05 8.458433214E-05 1.549654771E-05
4.415996524E-05-8.875497467E-05 4.629615556E-05-3.819301250E-05 2.973477708E-05
-4.032341081E-05 2.053537074E-06-2.175546998E-05-2.889234070E-05-2.061518169E-05
-7.859289894E-06 2.348711881E-05-8.277858560E-06 3.330293580E-06-2.905037155E-06
2.588223880E-06 8.204743128E-06-2.038129562E-05 7.589073593E-06 2.172056748E-06
-8.064004408E-07 1.082256860E-06 3.946550164E-06 1.228649380E-05 1.137214217E-05
-8.611316242E-06 8.817441634E-06 4.919801255E-06-1.772779193E-06-5.574806496E-06
-1.929934388E-06 1.568499330E-06 1.020905441E-05 2.510431467E-06 8.618821952E-06
-2.023283747E-06 1.361713779E-05-2.225972299E-06-1.159182059E-06 6.612606610E-06
-3.319925186E-06 2.487194851E-07-9.575865517E-06 1.198457509E-05
7.759761076E-01 9.771484255E-01-1.059298930E+00
......END OF GEOMETRY SEARCH......
STEP CPU TIME =     0.20 TOTAL CPU TIME =    13018.2 (  217.0 MIN)
TOTAL WALL CLOCK TIME=    19128.7 SECONDS, CPU UTILIZATION IS  68.06%
1342175  WORDS OF DYNAMIC MEMORY USED
EXECUTION OF GAMESS TERMINATED NORMALLY Wed Feb 21 16:36:49 2007
DDI: 262808 bytes (0.3 MB / 0 MWords) used by master data server.
```

Trans 3-(trimethylsilyl)-propionate

```
ECHO OF THE FIRST FEW INPUT CARDS -
INPUT CARD> $CONTRL RUNTYP=OPTIMIZE $END
INPUT CARD> $DFT DFTTYP=B3LYP $END
INPUT CARD> $BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.T. $END
INPUT CARD> $CONTRL ICHARG=-1 $END
INPUT CARD> $SYSTEM BALTYP=LOOP $END
INPUT CARD> $CONTRL MAXIT=30 $END
INPUT CARD> $SYSTEM TIMLIM=1200 MWORDS=62.50 $END
INPUT CARD>
INPUT CARD> $DATA
INPUT CARD>untitled
INPUT CARD>C1
INPUT CARD> C           6.0  -0.7106708961  -0.4720689079   0.5044196797
INPUT CARD> C           6.0  -1.6907748247  -0.2065207977  -0.6533422414
INPUT CARD> C           6.0  -3.0193421323  -1.0477830810  -0.5983663589
INPUT CARD> SI         14.0   1.0219411583   0.2484128099   0.3219836191
INPUT CARD> C           6.0   0.9790184542   2.1514081680   0.2108175221
INPUT CARD> C           6.0   1.8974450251  -0.4232406373  -1.2321289225
INPUT CARD> C           6.0   2.0850566170  -0.1982557724   1.8463427338
INPUT CARD> O           8.0  -2.9742214293  -2.1257032602   0.0542265094
INPUT CARD> O           8.0  -3.9796261059  -0.5570214101  -1.2515311458
INPUT CARD> H           1.0  -0.6421078423  -1.5600177327   0.6422046149
INPUT CARD> H           1.0  -1.1476088769  -0.0971433074   1.4433985739
INPUT CARD> H           1.0  -1.2182355842  -0.4508508546  -1.6170734170
INPUT CARD> H           1.0  -1.9666659303   0.8541454488  -0.7107563465
INPUT CARD> H           1.0   0.5658199179   2.5768344024   1.1345571081
INPUT CARD> H           1.0   0.3425462844   2.4823589938  -0.6176828771
INPUT CARD> H           1.0   1.9796609208   2.5802346950   0.0645168733
INPUT CARD> H           1.0   2.9379063326  -0.0800292110  -1.2892526715
INPUT CARD> H           1.0   1.3785893600  -0.0980473130  -2.1408865220
INPUT CARD> H           1.0   1.9002661443  -1.5203951372  -1.2295548867
INPUT CARD> H           1.0   3.0677214638   0.2915151373   1.8120343345
INPUT CARD> H           1.0   2.2473253976  -1.2802378157   1.9175792976
INPUT CARD> H           1.0   1.5801815459   0.1246775830   2.7649165227
INPUT CARD> $END
62000000 WORDS OF MEMORY AVAILABLE


NSERCH=  0     ENERGY=    -676.2566015

-----------------------
GRADIENT (HARTREE/BOHR)
-----------------------
ATOM            ZNUC       DE/DX         DE/DY         DE/DZ
------------------------------------------------------------
1  C            6.0    -0.0000115     0.0000332     0.0000440
2  C            6.0     0.0000090    -0.0000320     0.0000195
3  C            6.0     0.0000260    -0.0000243     0.0000181
4  SI          14.0    -0.0000133    -0.0000667    -0.0000049
5  C            6.0     0.0000176     0.0000336    -0.0000070
6  C            6.0     0.0000287     0.0000604     0.0000340
7  C            6.0    -0.0000072     0.0000212    -0.0000085
8  O            8.0     0.0000038    -0.0000260     0.0000231
9  O            8.0    -0.0000417     0.0000325    -0.0000270
10  H           1.0     0.0000044    -0.0000125    -0.0000214
11  H           1.0     0.0000068     0.0000022    -0.0000168
12  H           1.0     0.0000072     0.0000176    -0.0000299
13  H           1.0     0.0000097     0.0000028    -0.0000140
14  H           1.0     0.0000021     0.0000051     0.0000073
15  H           1.0     0.0000055     0.0000144    -0.0000028
16  H           1.0    -0.0000033    -0.0000012     0.0000023
17  H           1.0    -0.0000063    -0.0000151    -0.0000005
18  H           1.0    -0.0000226    -0.0000267    -0.0000019
19  H           1.0    -0.0000145    -0.0000017    -0.0000131
20  H           1.0     0.0000077    -0.0000001    -0.0000012
21  H           1.0     0.0000048    -0.0000085     0.0000040
22  H           1.0    -0.0000130    -0.0000081    -0.0000031
```

MAXIMUM GRADIENT = 0.0000667 RMS GRADIENT = 0.0000208

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.7106708961	-0.4720689079	0.5044196797
C	6.0	-1.6907748247	-0.2065207977	-0.6533422414
C	6.0	-3.0193421323	-1.0477830810	-0.5983663589
SI	14.0	1.0219411583	0.2484128099	0.3219836191
C	6.0	0.9790184542	2.1514081680	0.2108175221
C	6.0	1.8974450251	-0.4232406373	-1.2321289225
C	6.0	2.0850566170	-0.1982557724	1.8463427338
O	8.0	-2.9742214293	-2.1257032602	0.0542265094
O	8.0	-3.9796261059	-0.5570214101	-1.2515311458
H	1.0	-0.6421078423	-1.5600177327	0.6422046149
H	1.0	-1.1476088769	-0.0971433074	1.4433985739
H	1.0	-1.2182355842	-0.4508508546	-1.6170734170
H	1.0	-1.9666659303	0.8541454488	-0.7107563465
H	1.0	0.5658199179	2.5768344024	1.1345571081
H	1.0	0.3425462844	2.4823589938	-0.6176828771
H	1.0	1.9796609208	2.5802346950	0.0645168733
H	1.0	2.9379063326	-0.0800292110	-1.2892526715
H	1.0	1.3785893600	-0.0980473130	-2.1408865220
H	1.0	1.9002661443	-1.5203951372	-1.2295548867
H	1.0	3.0677214638	0.2915151373	1.8120343345
H	1.0	2.2473253976	-1.2802378157	1.9175792976
H	1.0	1.5801815459	0.1246775830	2.7649165227

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1 C	6.631384	-0.631384	6.509096	-0.509096
2 C	6.213961	-0.213961	6.336458	-0.336458
3 C	5.707664	0.292336	5.846804	0.153196
4 SI	12.927786	1.072214	13.452606	0.547394
5 C	6.711153	-0.711153	6.684677	-0.684677
6 C	6.738707	-0.738707	6.673518	-0.673518
7 C	6.699874	-0.699874	6.679569	-0.679569
8 O	8.617427	-0.617427	8.550512	-0.550512
9 O	8.628380	-0.628380	8.549055	-0.549055
10 H	0.820359	0.179641	0.797454	0.202546
11 H	0.869559	0.130441	0.818388	0.181612
12 H	0.882444	0.117556	0.827598	0.172402
13 H	0.864904	0.135096	0.828210	0.171790
14 H	0.856507	0.143493	0.825858	0.174142
15 H	0.837469	0.162531	0.818689	0.181311
16 H	0.866264	0.133736	0.834221	0.165779
17 H	0.866107	0.133893	0.834252	0.165748
18 H	0.840996	0.159004	0.820234	0.179766
19 H	0.848273	0.151727	0.824801	0.175199
20 H	0.865248	0.134752	0.833392	0.166608
21 H	0.852433	0.147567	0.828527	0.171473
22 H	0.853102	0.146898	0.826081	0.173919

BOND ORDER AND VALENCE ANALYSIS BOND ORDER THRESHOLD=0.050

ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER
1	2	1.540	0.845	1	4	1.885	0.897	1	8	2.839	0.110
1	10	1.099	0.952	1	11	1.101	0.932	2	3	1.573	0.968
2	8	2.415	-0.231	2	9	2.392	-0.069	2	12	1.101	0.945
2	13	1.097	0.909	3	8	1.261	1.648	3	9	1.261	1.612
3	13	2.177	0.065	4	5	1.907	0.819	4	6	1.906	0.859
4	7	1.911	0.755	5	14	1.098	0.970	5	15	1.096	0.977
5	16	1.098	0.971	6	17	1.097	0.974	6	18	1.096	0.976
6	19	1.097	0.972	7	20	1.098	0.970	7	21	1.096	0.976
7	22	1.097	0.975								

ATOM	TOTAL VALENCE	BONDED VALENCE	FREE VALENCE
1 C	3.646	3.646	0.000
2 C	3.258	3.258	0.000
3 C	4.402	4.402	0.000
4 SI	3.273	3.273	0.000
5 C	3.633	3.633	0.000
6 C	3.712	3.712	0.000
7 C	3.601	3.601	0.000
8 O	1.554	1.554	0.000
9 O	1.529	1.529	0.000
10 H	0.944	0.944	0.000
11 H	0.946	0.946	0.000
12 H	0.946	0.946	0.000
13 H	0.947	0.947	0.000
14 H	0.951	0.951	0.000
15 H	0.948	0.948	0.000
16 H	0.952	0.952	0.000
17 H	0.952	0.952	0.000
18 H	0.949	0.949	0.000
19 H	0.950	0.950	0.000
20 H	0.952	0.952	0.000
21 H	0.952	0.952	0.000
22 H	0.951	0.951	0.000

```
NUCLEAR ENERGY    =      523.3640832421
ELECTRONIC ENERGY =    -1199.6206847243
TOTAL ENERGY      =     -676.2566014823

THE INITIAL GEOMETRY IS ALREADY CONVERGED,
SO ORBITALS/PROPERTY OUTPUT IS ALREADY PRINTED ABOVE
$VIB
IVIB=   0 IATOM=   0 ICOORD=   0 E=     -676.2566014823
-1.151548435E-05 3.321499759E-05 4.404164183E-05 8.990855241E-06-3.195747925E-05
1.951764813E-05 2.595023447E-05-2.434090715E-05 1.810238763E-05-1.330157170E-05
-6.666436059E-05-4.896055931E-06 1.761547449E-05 3.361839130E-05-7.035438705E-06
2.871354044E-05 6.036985112E-05 3.395249682E-05-7.186430447E-06 2.116890822E-05
-8.488270752E-06 3.766137356E-06-2.598354889E-05 2.311121529E-05-4.166038004E-05
3.248780601E-05-2.698555409E-05 4.405198594E-06-1.251727549E-05-2.138230824E-05
6.772363948E-06 2.179335584E-06-1.680275930E-05 7.206362876E-06 1.757563936E-05
-2.988288107E-05 9.691130807E-06 2.781019356E-06-1.403745685E-05 2.136466323E-06
5.076646562E-06 7.295341002E-06 5.502809244E-06 1.443994401E-05-2.795530553E-06
-3.309766219E-06-1.242749607E-06 2.295175327E-06-6.279152946E-06-1.506240148E-05
-5.212806127E-07-2.256015459E-05-2.669052121E-05-1.936414905E-06-1.446828370E-05
-1.732300466E-06-1.314768053E-05 7.713121287E-06-1.482111068E-07-1.240934657E-06
4.802095876E-06-8.462893188E-06 3.984966642E-06-1.298456695E-05-8.109890679E-06
-3.148306482E-06
1.225524258E+01 4.569315876E+00 2.258489650E+00
......END OF GEOMETRY SEARCH......
STEP CPU TIME =     0.22 TOTAL CPU TIME =     1417.8 (   23.6 MIN)
TOTAL WALL CLOCK TIME=     2576.0 SECONDS, CPU UTILIZATION IS  55.04%
1326317  WORDS OF DYNAMIC MEMORY USED
EXECUTION OF GAMESS TERMINATED NORMALLY Sat Mar 24 18:14:39 2007
DDI: 262808 bytes (0.3 MB / 0 MWords) used by master data server.
```

Gauche 4,4-dimethylpentanoic acid

```
ECHO OF THE FIRST FEW INPUT CARDS -
INPUT CARD> $CONTRL RUNTYP=OPTIMIZE $END
INPUT CARD> $DFT DFTTYP=B3LYP $END
INPUT CARD> $BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.T. $END
INPUT CARD> $SYSTEM BALTYP=LOOP $END
INPUT CARD> $SYSTEM TIMLIM=600 MWORDS=18.75 $END
INPUT CARD>
INPUT CARD> $DATA
INPUT CARD>untitled
INPUT CARD>C1
INPUT CARD> C           6.0  -0.8362349321  -0.2786619210   0.6099115648
INPUT CARD> C           6.0  -1.7571339913   0.2278196838  -0.5217922074
INPUT CARD> C           6.0   0.6485583830   0.1806042746   0.5855227757
INPUT CARD> C           6.0   0.7495944892   1.7136509414   0.7257765144
INPUT CARD> C           6.0   1.3544703962  -0.2648237067  -0.7116131649
INPUT CARD> C           6.0   1.3550388579  -0.4816126018   1.7867677183
INPUT CARD> H           1.0  -0.8704553410  -1.3740723172   0.6281292302
INPUT CARD> H           1.0  -1.2730027828   0.0576232464   1.5594110332
INPUT CARD> C           6.0  -1.6458846391  -0.4713502499  -1.8586013787
INPUT CARD> H           1.0   0.2084737196   2.0680291201   1.6120534234
INPUT CARD> H           1.0   0.3483615654   2.2358346522  -0.1496884206
INPUT CARD> H           1.0   1.7968122440   2.0211470809   0.8309588790
INPUT CARD> H           1.0   2.4140287382   0.0182608213  -0.6890052342
INPUT CARD> H           1.0   0.9171534366   0.2054849548  -1.5988458155
INPUT CARD> H           1.0   1.3015606064  -1.3520288107  -0.8384072252
INPUT CARD> H           1.0   2.4107104350  -0.1877809511   1.8312494179
INPUT CARD> H           1.0   1.3154385510  -1.5746655644   1.7134125328
INPUT CARD> H           1.0   0.8908669947  -0.1928313009   2.7380398683
INPUT CARD> H           1.0  -1.6291571555   1.2946444524  -0.7127083886
INPUT CARD> H           1.0  -2.7992962722   0.0860162767  -0.2042971416
INPUT CARD> O           8.0  -1.6782521698  -1.8267297873  -1.7458910845
INPUT CARD> O           8.0  -1.5836906544   0.0771995912  -2.9401702677
INPUT CARD> H           1.0  -1.6379674787  -2.1817678846  -2.6502126289
INPUT CARD> $END
18000000 WORDS OF MEMORY AVAILABLE

NSERCH= 10     ENERGY=    -425.4238637

-----------------------
GRADIENT (HARTREE/BOHR)
-----------------------
ATOM            ZNUC       DE/DX         DE/DY         DE/Z
------------------------------------------------------------
1  C            6.0    -0.0000378    -0.0000310     0.0000450
2  C            6.0     0.0000364     0.0000262    -0.0000021
3  C            6.0    -0.0000242    -0.0000051    -0.0000061
4  C            6.0     0.0000077    -0.0000452    -0.0000100
5  C            6.0     0.0000469     0.0000121     0.0000197
6  C            6.0    -0.0000201     0.0000301     0.0000066
7  H            1.0    -0.0000003     0.0000061    -0.0000264
8  H            1.0     0.0000202     0.0000139    -0.0000049
9  C            6.0    -0.0000046     0.0000576     0.0000017
10  H           1.0    -0.0000216     0.0000055     0.0000165
11  H           1.0    -0.0000035     0.0000105    -0.0000239
12  H           1.0     0.0000128     0.0000028     0.0000034
13  H           1.0    -0.0000083    -0.0000020     0.0000071
14  H           1.0     0.0000277     0.0000083    -0.0000216
15  H           1.0     0.0000054    -0.0000136     0.0000064
16  H           1.0     0.0000051    -0.0000097    -0.0000163
17  H           1.0     0.0000124     0.0000011    -0.0000141
18  H           1.0    -0.0000111    -0.0000043    -0.0000051
19  H           1.0    -0.0000201     0.0000043     0.0000111
20  H           1.0    -0.0000172     0.0000096     0.0000205
21  O           8.0     0.0000114    -0.0000493    -0.0000244
22  O           8.0    -0.0000114    -0.0000083     0.0000054
23  H           1.0    -0.0000058    -0.0000197     0.0000115

MAXIMUM GRADIENT =  0.0000576    RMS GRADIENT = 0.0000200
```

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.8352681876	-0.2735469353	0.6038619811
C	6.0	-1.7504293277	0.2311508425	-0.5335191827
C	6.0	0.6497257579	0.1848092097	0.5854938698
C	6.0	0.7512860521	1.7162825073	0.7400792551
C	6.0	1.3577430895	-0.2484182017	-0.7147147942
C	6.0	1.3538284360	-0.4872704117	1.7824610459
H	1.0	-0.8705039259	-1.3688402590	0.6237918961
H	1.0	-1.2755328780	0.0643283256	1.5512325305
C	6.0	-1.6463381318	-0.4878874305	-1.8603282150
H	1.0	0.2221381695	2.0600160736	1.6379818231
H	1.0	0.3348595759	2.2476295478	-0.1226055372
H	1.0	1.7993115753	2.0240358373	0.8335309578
H	1.0	2.4185249659	0.0290752116	-0.6846165603
H	1.0	0.9246685891	0.2332799017	-1.5977207856
H	1.0	1.3014558877	-1.3341954266	-0.8529982888
H	1.0	2.4082179686	-0.1905286223	1.8343830633
H	1.0	1.3190296022	-1.5798280130	1.6960566854
H	1.0	0.8836832984	-0.2112976328	2.7345899294
H	1.0	-1.6094089474	1.2945104562	-0.7375906136
H	1.0	-2.7945234528	0.1050022798	-0.2147776478
O	8.0	-1.7048472117	-1.8408712196	-1.7282778847
O	8.0	-1.5689870540	0.0437503360	-2.9496418392
H	1.0	-1.6686408513	-2.2111963765	-2.6266716883

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1 C	6.153107	-0.153107	6.323481	-0.323481
2 C	6.233312	-0.233312	6.283385	-0.283385
3 C	5.740037	0.259963	6.226971	-0.226971
4 C	6.529099	-0.529099	6.448145	-0.448145
5 C	6.516078	-0.516078	6.438684	-0.438684
6 C	6.480527	-0.480527	6.447062	-0.447062
7 H	0.840475	0.159525	0.805114	0.194886
8 H	0.864964	0.135036	0.818129	0.181871
9 C	5.838743	0.161257	5.793081	0.206919
10 H	0.856815	0.143185	0.823018	0.176982
11 H	0.855024	0.144976	0.822481	0.177519
12 H	0.852584	0.147416	0.825656	0.174344
13 H	0.854951	0.145049	0.825498	0.174502
14 H	0.841317	0.158683	0.810017	0.189983
15 H	0.852121	0.147879	0.820046	0.179954
16 H	0.853475	0.146525	0.827689	0.172311
17 H	0.853183	0.146817	0.826785	0.173215
18 H	0.855624	0.144376	0.825605	0.174395
19 H	0.832153	0.167847	0.800671	0.199329
20 H	0.828003	0.171997	0.804322	0.195678
21 O	8.411088	-0.411088	8.365140	-0.365140
22 O	8.422569	-0.422569	8.355360	-0.355360
23 H	0.634752	0.365248	0.683663	0.316337

BOND ORDER AND VALENCE ANALYSIS BOND ORDER THRESHOLD=0.050

ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER
1	2	1.545	0.958	1	3	1.554	0.843	1	6	2.495	-0.059
1	7	1.096	0.954	1	8	1.098	0.960	1	9	2.603	-0.131
2	3	2.649	-0.052	2	9	1.513	0.995	2	19	1.092	0.977
2	20	1.099	0.930	2	21	2.392	-0.256	2	22	2.430	-0.153
3	4	1.543	0.839	3	5	1.543	0.802	3	6	1.543	0.792
3	16	2.189	-0.052	4	10	1.097	1.002	4	11	1.095	1.000
4	12	1.096	1.001	5	13	1.097	1.004	5	14	1.095	0.988
5	15	1.096	0.997	6	16	1.097	1.013	6	17	1.097	1.014

```
6     18  1.097  1.002        9  21  1.361  1.245        9  22  1.215  2.057
21    22  2.250 -0.053       21  23  0.972  0.798

                     TOTAL       BONDED        FREE
ATOM                VALENCE     VALENCE     VALENCE
1 C                  3.502       3.502       0.000
2 C                  3.376       3.376       0.000
3 C                  2.943       2.943       0.000
4 C                  3.737       3.737       0.000
5 C                  3.673       3.673       0.000
6 C                  3.595       3.595       0.000
7 H                  0.940       0.940       0.000
8 H                  0.944       0.944       0.000
9 C                  4.299       4.299       0.000
10 H                 0.946       0.946       0.000
11 H                 0.946       0.946       0.000
12 H                 0.946       0.946       0.000
13 H                 0.945       0.945       0.000
14 H                 0.944       0.944       0.000
15 H                 0.944       0.944       0.000
16 H                 0.946       0.946       0.000
17 H                 0.944       0.944       0.000
18 H                 0.945       0.945       0.000
19 H                 0.940       0.940       0.000
20 H                 0.935       0.935       0.000
21 O                 1.755       1.755       0.000
22 O                 1.845       1.845       0.000
23 H                 0.866       0.866       0.000

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ELECTROSTATIC MOMENTS
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POINT   1           X           Y           Z (BOHR)    CHARGE
-0.731757   -0.289812   -0.922011        0.00 (A.U.)
DX          DY          DZ         /D/  (DEBYE)
0.059041   -0.813705    1.716225    1.900271
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =     3.28 TOTAL CPU TIME =    16697.8 (  278.3 MIN)
TOTAL WALL CLOCK TIME=    29227.4 SECONDS, CPU UTILIZATION IS  57.13%
$VIB
IVIB=   0 IATOM=   0 ICOORD=   0 E=     -425.4238637398
-3.779084347E-05-3.097226894E-05 4.504006438E-05 3.635877397E-05 2.617739722E-05
-2.086324591E-06-2.422857034E-05-5.102406841E-06-6.089643966E-06 7.718046201E-06
-4.521781057E-05-1.000109040E-05 4.687270734E-05 1.211882311E-05 1.974720327E-05
-2.005541421E-05 3.012547160E-05 6.579217113E-06-3.437824385E-07 6.076842438E-06
-2.641263451E-05 2.023817408E-05 1.385091166E-05-4.927959996E-06-4.622608856E-06
5.760433261E-05 1.686534489E-06-2.158989622E-05 5.485353583E-06 1.645868177E-05
-3.516494819E-06 1.049238060E-05-2.391828698E-05 1.284618988E-05 2.847625705E-06
3.376645785E-06-8.301999088E-06-1.988736387E-06 7.098341424E-06 2.772660540E-05
8.297736660E-06-2.158102045E-05 5.436115178E-06-1.356290945E-05 6.417708685E-06
5.081367718E-06-9.685785871E-06-1.626005876E-05 1.244203129E-05 1.092189417E-06
-1.413791167E-05-1.105210142E-05-4.341057256E-06-5.125183889E-06-2.012053307E-05
4.310414041E-06 1.108772296E-05-1.724179159E-05 9.648175866E-06 2.051592706E-05
1.142025592E-05-4.928784499E-05-2.437952132E-05-1.142681521E-05-8.275008978E-06
5.387292080E-06-5.849416232E-06-1.969382523E-05 1.152429752E-05
5.904092838E-02-8.137049050E-01 1.716225370E+00
......END OF GEOMETRY SEARCH......
STEP CPU TIME =     0.22 TOTAL CPU TIME =    16698.0 (  278.3 MIN)
TOTAL WALL CLOCK TIME=    29227.6 SECONDS, CPU UTILIZATION IS  57.13%
1324465  WORDS OF DYNAMIC MEMORY USED
EXECUTION OF GAMESS TERMINATED NORMALLY Mon Feb 26 19:42:42 2007
DDI: 262808 bytes (0.3 MB / 0 MWords) used by master data server.
```

Gauche 4,4-dimethylpentanoate

```
ECHO OF THE FIRST FEW INPUT CARDS -
INPUT CARD> $CONTRL RUNTYP=OPTIMIZE $END
INPUT CARD> $DFT DFTTYP=B3LYP $END
INPUT CARD> $BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.T. $END
INPUT CARD> $CONTRL ICHARG=-1 $END
INPUT CARD> $SYSTEM BALTYP=LOOP $END
INPUT CARD> $CONTRL MAXIT=30 $END
INPUT CARD> $SYSTEM TIMLIM=1200 MWORDS=62.50 $END
INPUT CARD>
INPUT CARD> $DATA
INPUT CARD>untitled
INPUT CARD>C1
INPUT CARD>C        6.0       -0.835270       -0.273549        0.603861
INPUT CARD>C        6.0       -1.750430        0.231151       -0.533519
INPUT CARD>C        6.0        0.649730        0.184811        0.585491
INPUT CARD>C        6.0        0.751290        1.716281        0.740081
INPUT CARD>C        6.0        1.357740       -0.248419       -0.714709
INPUT CARD>C        6.0        1.353830       -0.487269        1.782461
INPUT CARD>H        1.0       -0.870500       -1.368839        0.623791
INPUT CARD>H        1.0       -1.275530        0.064331        1.551231
INPUT CARD>C        6.0       -1.646340       -0.487889       -1.860329
INPUT CARD>H        1.0        0.222140        2.060021        1.637981
INPUT CARD>H        1.0        0.334860        2.247631       -0.122609
INPUT CARD>H        1.0        1.799310        2.024041        0.833531
INPUT CARD>H        1.0        2.418520        0.029081       -0.684619
INPUT CARD>H        1.0        0.924670        0.233281       -1.597719
INPUT CARD>H        1.0        1.301460       -1.334199       -0.852999
INPUT CARD>H        1.0        2.408220       -0.190529        1.834381
INPUT CARD>H        1.0        1.319030       -1.579829        1.696061
INPUT CARD>H        1.0        0.883680       -0.211299        2.734591
INPUT CARD>H        1.0       -1.609410        1.294511       -0.737589
INPUT CARD>H        1.0       -2.794520        0.105001       -0.214779
INPUT CARD>O        8.0       -1.704850       -1.840869       -1.728279
INPUT CARD>O        8.0       -1.568990        0.043751       -2.949639
INPUT CARD> $END
62000000 WORDS OF MEMORY AVAILABLE


NSERCH= 19     ENERGY=    -424.8671417

-----------------------
GRADIENT (HARTREE/BOHR)
-----------------------
ATOM           ZNUC       DE/DX         DE/DY         DE/DZ
------------------------------------------------------------
1  C            6.0    -0.0000038     0.0000150    -0.0000039
2  C            6.0    -0.0000207     0.0000069     0.0000428
3  C            6.0     0.0000191    -0.0000146     0.0000464
4  C            6.0     0.0000252     0.0000205    -0.0000076
5  C            6.0     0.0000097     0.0000087    -0.0000145
6  C            6.0    -0.0000302    -0.0000223    -0.0000079
7  H            1.0    -0.0000114     0.0000116    -0.0000033
8  H            1.0     0.0000114     0.0000096    -0.0000132
9  C            6.0    -0.0000206    -0.0000800    -0.0000258
10  H           1.0     0.0000108    -0.0000168    -0.0000329
11  H           1.0     0.0000025     0.0000049     0.0000304
12  H           1.0    -0.0000289    -0.0000047     0.0000097
13  H           1.0    -0.0000097     0.0000009    -0.0000014
14  H           1.0     0.0000059    -0.0000103     0.0000088
15  H           1.0     0.0000135    -0.0000033     0.0000032
16  H           1.0    -0.0000001    -0.0000016     0.0000036
17  H           1.0    -0.0000001     0.0000185    -0.0000150
18  H           1.0     0.0000088     0.0000083    -0.0000131
19  H           1.0     0.0000017     0.0000057     0.0000059
20  H           1.0     0.0000002    -0.0000122    -0.0000047
21  O           8.0     0.0000117     0.0000741    -0.0000096
22  O           8.0     0.0000048    -0.0000190     0.0000019
```

MAXIMUM GRADIENT = 0.0000800 RMS GRADIENT = 0.0000204

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.8612346726	-0.2210079126	0.6092568397
C	6.0	-1.7218685827	0.2362062198	-0.5807602395
C	6.0	0.6374522871	0.1993324374	0.6001335930
C	6.0	0.7778503852	1.7235618221	0.7972607686
C	6.0	1.3181200465	-0.2087565563	-0.7226858579
C	6.0	1.3454513385	-0.5132762541	1.7718040970
H	1.0	-0.9127749847	-1.3168446656	0.6304798471
H	1.0	-1.2938373911	0.1429420312	1.5573038962
C	6.0	-1.6141934843	-0.6623337250	-1.8637380607
H	1.0	0.3599862496	2.0375089181	1.7636087070
H	1.0	0.2545989524	2.2765246819	0.0103192743
H	1.0	1.8337686187	2.0277415570	0.7732617039
H	1.0	2.3903248317	0.0377920658	-0.6975210877
H	1.0	0.8679765205	0.3089535368	-1.5746349000
H	1.0	1.2043205408	-1.2816126445	-0.9046349191
H	1.0	2.4045546596	-0.2242909626	1.8342749499
H	1.0	1.2998424718	-1.6017560571	1.6470399992
H	1.0	0.8728248737	-0.2647554838	2.7320822947
H	1.0	-1.5291071528	1.2800329099	-0.8566980452
H	1.0	-2.7787446169	0.1907294330	-0.2769672297
O	8.0	-1.5129791926	-1.9032746643	-1.6561753361
O	8.0	-1.6736916981	-0.0522146871	-2.9663382948

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1 C	6.174897	-0.174897	6.342749	-0.342749
2 C	6.311649	-0.311649	6.340097	-0.340097
3 C	5.574855	0.425145	6.233775	-0.233775
4 C	6.594998	-0.594998	6.466797	-0.466797
5 C	6.578973	-0.578973	6.446978	-0.446978
6 C	6.537099	-0.537099	6.466513	-0.466513
7 H	0.829961	0.170039	0.800169	0.199831
8 H	0.910990	0.089010	0.837782	0.162218
9 C	5.798015	0.201985	5.869646	0.130354
10 H	0.877519	0.122481	0.833590	0.166410
11 H	0.850443	0.149557	0.819602	0.180398
12 H	0.879692	0.120308	0.838089	0.161911
13 H	0.896395	0.103605	0.843492	0.156508
14 H	0.817042	0.182958	0.799456	0.200544
15 H	0.825451	0.174549	0.807200	0.192800
16 H	0.879003	0.120997	0.839115	0.160885
17 H	0.855539	0.144461	0.827686	0.172314
18 H	0.874369	0.125631	0.834000	0.166000
19 H	0.877722	0.122278	0.823726	0.176274
20 H	0.882405	0.117595	0.830481	0.169519
21 O	8.580302	-0.580302	8.552538	-0.552538
22 O	8.592681	-0.592681	8.546518	-0.546518

BOND ORDER AND VALENCE ANALYSIS BOND ORDER THRESHOLD=0.050

ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER
1	2	1.538	0.910	1	3	1.557	0.844	1	6	2.511	-0.062
1	7	1.097	0.953	1	8	1.104	0.971	1	9	2.622	-0.119
1	19	2.202	-0.060	1	20	2.152	-0.054	1	21	2.896	0.101
2	9	1.570	0.948	2	19	1.097	0.975	2	20	1.101	0.968
2	21	2.404	-0.259	2	22	2.403	-0.160	3	4	1.543	0.748
3	5	1.543	0.808	3	6	1.543	0.650	3	11	2.193	-0.058
3	13	2.187	-0.052	3	16	2.197	-0.070	3	17	2.186	-0.095
3	18	2.195	-0.075	3	21	3.760	-0.062	4	10	1.099	1.022
4	11	1.095	1.025	4	12	1.099	1.015	5	13	1.100	1.019

```
5     14  1.094  0.985        5  15  1.094  1.002        6  16  1.100  1.023
6     17  1.097  1.055        6  18  1.099  1.028        9  21  1.262  1.726
9     22  1.262  1.802

                      TOTAL       BONDED        FREE
ATOM                 VALENCE     VALENCE     VALENCE
1 C                   3.461       3.461       0.000
2 C                   3.347       3.347       0.000
3 C                   2.552       2.552       0.000
4 C                   3.742       3.742       0.000
5 C                   3.727       3.727       0.000
6 C                   3.533       3.533       0.000
7 H                   0.942       0.942       0.000
8 H                   0.949       0.949       0.000
9 C                   4.414       4.414       0.000
10 H                  0.949       0.949       0.000
11 H                  0.947       0.947       0.000
12 H                  0.949       0.949       0.000
13 H                  0.949       0.949       0.000
14 H                  0.940       0.940       0.000
15 H                  0.940       0.940       0.000
16 H                  0.949       0.949       0.000
17 H                  0.946       0.946       0.000
18 H                  0.949       0.949       0.000
19 H                  0.947       0.947       0.000
20 H                  0.946       0.946       0.000
21 O                  1.528       1.528       0.000
22 O                  1.555       1.555       0.000

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ELECTROSTATIC MOMENTS
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POINT   1           X           Y           Z (BOHR)    CHARGE
-0.693564   -0.307293   -0.877025       -1.00 (A.U.)
DX          DY          DZ         /D/  (DEBYE)
4.573109    3.403337    7.752122    9.622444
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =     3.13 TOTAL CPU TIME =    26505.6 (  441.8 MIN)
TOTAL WALL CLOCK TIME=    63715.9 SECONDS, CPU UTILIZATION IS  41.60%
$VIB
IVIB=   0 IATOM=   0 ICOORD=   0 E=     -424.8671416613
-3.835520095E-06 1.500188985E-05-3.856503333E-06-2.070232477E-05 6.885661966E-06
4.284881454E-05 1.913774502E-05-1.460908379E-05 4.644338513E-05 2.518889154E-05
2.046693939E-05-7.577778467E-06 9.722010142E-06 8.683052501E-06-1.445819998E-05
-3.018545219E-05-2.230012854E-05-7.936184602E-06-1.140779160E-05 1.161849408E-05
-3.257407276E-06 1.142177169E-05 9.554228692E-06-1.322008249E-05-2.055179816E-05
-8.003904953E-05-2.584862562E-05 1.082077100E-05-1.678969837E-05-3.292001040E-05
2.462744622E-06 4.907065278E-06 3.040506985E-05-2.887628508E-05-4.669905343E-06
9.708029616E-06-9.730674044E-06 9.423129433E-07-1.366582744E-06 5.891934050E-06
-1.025746593E-05 8.797769777E-06 1.350473535E-05-3.274886952E-06 3.151680828E-06
-8.893969624E-08-1.637947122E-06 3.585832614E-06-5.027376090E-08 1.847769538E-05
-1.495397128E-05 8.814693966E-06 8.307259229E-06-1.306782197E-05 1.691487974E-06
5.746248804E-06 5.877421650E-06 2.085075395E-07-1.218706261E-05-4.698415891E-06
1.174570612E-05 7.412464446E-05-9.573383704E-06 4.818060372E-06-1.895026439E-05
1.916963751E-06
4.573109472E+00 3.403336861E+00 7.752122009E+00
......END OF GEOMETRY SEARCH......
STEP CPU TIME =     0.20 TOTAL CPU TIME =    26505.8 (  441.8 MIN)
TOTAL WALL CLOCK TIME=    63716.1 SECONDS, CPU UTILIZATION IS  41.60%
1309083  WORDS OF DYNAMIC MEMORY USED
EXECUTION OF GAMESS TERMINATED NORMALLY Mon Apr  2 09:13:23 2007
DDI: 262808 bytes (0.3 MB / 0 MWords) used by master data server.
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Trans 4,4-dimethylpentanoic acid

```
ECHO OF THE FIRST FEW INPUT CARDS -
INPUT CARD> $CONTRL RUNTYP=OPTIMIZE $END
INPUT CARD> $DFT DFTTYP=B3LYP $END
INPUT CARD> $BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.T. $END
INPUT CARD> $SYSTEM BALTYP=LOOP $END
INPUT CARD> $SYSTEM TIMLIM=900 MWORDS=31.25 $END
INPUT CARD>
INPUT CARD> $DATA
INPUT CARD>untitled
INPUT CARD>C1
INPUT CARD> C           6.0  -0.4186496877  -0.4364266731   0.4665036814
INPUT CARD> C           6.0  -1.4299258804  -0.1771629947  -0.6554517016
INPUT CARD> C           6.0  -2.7335423409  -0.9202754727  -0.4668632404
INPUT CARD> C           6.0   0.9712956309   0.2342920422   0.2934928040
INPUT CARD> C           6.0   0.8344261569   1.7663592435   0.1888937022
INPUT CARD> C           6.0   1.6957719301  -0.3123032096  -0.9542859193
INPUT CARD> C           6.0   1.8199585418  -0.1119805584   1.5348848214
INPUT CARD> O           8.0  -2.9689882972  -1.7714366910   0.3649477831
INPUT CARD> O           8.0  -3.6650093309  -0.5265429884  -1.3786045538
INPUT CARD> H           1.0  -0.2795012534  -1.5188418855   0.5734771944
INPUT CARD> H           1.0  -0.8574092104  -0.0992181190   1.4148002749
INPUT CARD> H           1.0  -1.0368661701  -0.4819808643  -1.6336947163
INPUT CARD> H           1.0  -1.6754112467   0.8859071890  -0.7553722630
INPUT CARD> H           1.0   0.2952502259   2.1774238457   1.0512776040
INPUT CARD> H           1.0   0.2982668852   2.0678803117  -0.7182971517
INPUT CARD> H           1.0   1.8197980016   2.2472688451   0.1562134346
INPUT CARD> H           1.0   2.7105438685   0.0969098951  -1.0236665260
INPUT CARD> H           1.0   1.1827229647  -0.0547396873  -1.8886246628
INPUT CARD> H           1.0   1.7817103783  -1.4053746270  -0.9097996109
INPUT CARD> H           1.0   2.8183082586   0.3353747270   1.4593012239
INPUT CARD> H           1.0   1.9463471280  -1.1965765422   1.6378025016
INPUT CARD> H           1.0   1.3555317110   0.2566778089   2.4581009160
INPUT CARD> H           1.0  -4.4646292636  -1.0552335950  -1.2150355959
INPUT CARD> $END
31000000 WORDS OF MEMORY AVAILABLE


NSERCH= 18     ENERGY=    -425.4260568

-----------------------
GRADIENT (HARTREE/BOHR)
-----------------------
ATOM             ZNUC       DE/DX         DE/DY         DE/DZ
------------------------------------------------------------
1  C            6.0     0.0000194     0.0000111    -0.0000501
2  C            6.0     0.0000301    -0.0000624     0.0000122
3  C            6.0    -0.0000018    -0.0000598     0.0000076
4  C            6.0    -0.0000496     0.0000291     0.0000700
5  C            6.0     0.0000460    -0.0000065    -0.0000802
6  C            6.0    -0.0000103    -0.0000085     0.0000159
7  C            6.0     0.0000181    -0.0000735    -0.0000276
8  O            8.0     0.0000305     0.0000607    -0.0000182
9  O            8.0    -0.0000027     0.0000384    -0.0000230
10  H            1.0    -0.0000350    -0.0000112    -0.0000109
11  H            1.0     0.0000224    -0.0000019     0.0000098
12  H            1.0    -0.0000059    -0.0000031     0.0000145
13  H            1.0    -0.0000166     0.0000420     0.0000234
14  H            1.0    -0.0000184     0.0000209     0.0000326
15  H            1.0    -0.0000571    -0.0000042    -0.0000016
16  H            1.0     0.0000003    -0.0000042     0.0000090
17  H            1.0     0.0000288     0.0000317    -0.0000128
18  H            1.0    -0.0000020    -0.0000076    -0.0000069
19  H            1.0     0.0000228    -0.0000297     0.0000074
20  H            1.0    -0.0000058     0.0000177     0.0000115
21  H            1.0    -0.0000084    -0.0000017     0.0000000
22  H            1.0    -0.0000053     0.0000251     0.0000021
23  H            1.0     0.0000006    -0.0000023     0.0000153
```

MAXIMUM GRADIENT = 0.0000802 RMS GRADIENT = 0.0000289

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.4336228590	-0.4042654387	0.4815962298
C	6.0	-1.4385410973	-0.1542871397	-0.6488120869
C	6.0	-2.7074633931	-0.9653892869	-0.5079409768
C	6.0	0.9657152495	0.2421321464	0.2992542858
C	6.0	0.8587227304	1.7760810258	0.1792590826
C	6.0	1.6766823355	-0.3303719241	-0.9447339647
C	6.0	1.8124579884	-0.1054346562	1.5413070108
O	8.0	-2.8697384102	-1.9379071669	0.1991369871
O	8.0	-3.6952441942	-0.4883604709	-1.3134307625
H	1.0	-0.3115676874	-1.4864657740	0.6072945106
H	1.0	-0.8699055709	-0.0424720084	1.4226526700
H	1.0	-1.0153524367	-0.4226914514	-1.6257071739
H	1.0	-1.7241255253	0.9001057463	-0.7272677450
H	1.0	0.3910151963	2.2107845450	1.0716236444
H	1.0	0.2683245082	2.0788210415	-0.6925869399
H	1.0	1.8527383374	2.2266752071	0.0725019604
H	1.0	2.7043643191	0.0454338514	-1.0107602602
H	1.0	1.1766268042	-0.0583756485	-1.8819871763
H	1.0	1.7272051922	-1.4257845906	-0.8981320822
H	1.0	2.8153200373	0.3305953622	1.4614263919
H	1.0	1.9266330443	-1.1906427051	1.6512268195
H	1.0	1.3532660494	0.2754539953	2.4621565992
H	1.0	-4.4635116179	-1.0736346596	-1.1980770239

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1 C	6.303424	-0.303424	6.318812	-0.318812
2 C	6.378693	-0.378693	6.289214	-0.289214
3 C	5.530578	0.469422	5.771492	0.228508
4 C	5.691122	0.308878	6.230560	-0.230560
5 C	6.520477	-0.520477	6.450687	-0.450687
6 C	6.527225	-0.527225	6.447040	-0.447040
7 C	6.447915	-0.447915	6.447796	-0.447796
8 O	8.469365	-0.469365	8.352643	-0.352643
9 O	8.457944	-0.457944	8.364406	-0.364406
10 H	0.836241	0.163759	0.806055	0.193945
11 H	0.854705	0.145295	0.811778	0.188222
12 H	0.826928	0.173072	0.797327	0.202673
13 H	0.828114	0.171886	0.802984	0.197016
14 H	0.854475	0.145525	0.821505	0.178495
15 H	0.859542	0.140458	0.824322	0.175678
16 H	0.853600	0.146400	0.825255	0.174745
17 H	0.852980	0.147020	0.825619	0.174381
18 H	0.861725	0.138275	0.826639	0.173361
19 H	0.852150	0.147850	0.823750	0.176250
20 H	0.855345	0.144655	0.827358	0.172642
21 H	0.852181	0.147819	0.826070	0.173930
22 H	0.854361	0.145639	0.824436	0.175564
23 H	0.630908	0.369092	0.684252	0.315748

BOND ORDER AND VALENCE ANALYSIS BOND ORDER THRESHOLD=0.050

ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER
1	2	1.533	0.922	1	4	1.552	0.927	1	7	2.501	-0.052
1	8	2.892	0.093	1	10	1.096	0.929	1	11	1.099	0.956
2	3	1.513	1.105	2	8	2.439	-0.111	2	9	2.376	0.086
2	12	1.098	0.915	2	13	1.095	0.938	3	8	1.213	1.845
3	9	1.361	0.843	4	5	1.542	0.814	4	6	1.543	0.819
4	7	1.543	0.743	4	21	2.192	-0.064	4	22	2.198	-0.066
5	7	2.511	-0.058	5	14	1.097	1.002	5	15	1.096	1.008

```
5     16  1.097  0.993        6  17  1.096  0.991        6  18  1.097  1.001
6     19  1.098  1.003        7  20  1.096  1.001        7  21  1.097  1.016
7     22  1.097  1.017        9  23  0.973  0.794
```

ATOM	TOTAL VALENCE	BONDED VALENCE	FREE VALENCE
1 C	3.805	3.805	0.000
2 C	3.785	3.785	0.000
3 C	3.900	3.900	0.000
4 C	2.932	2.932	0.000
5 C	3.716	3.716	0.000
6 C	3.737	3.737	0.000
7 C	3.519	3.519	0.000
8 O	1.854	1.854	0.000
9 O	1.727	1.727	0.000
10 H	0.940	0.940	0.000
11 H	0.942	0.942	0.000
12 H	0.939	0.939	0.000
13 H	0.939	0.939	0.000
14 H	0.945	0.945	0.000
15 H	0.945	0.945	0.000
16 H	0.946	0.946	0.000
17 H	0.945	0.945	0.000
18 H	0.947	0.947	0.000
19 H	0.944	0.944	0.000
20 H	0.946	0.946	0.000
21 H	0.944	0.944	0.000
22 H	0.945	0.945	0.000
23 H	0.857	0.857	0.000

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ELECTROSTATIC MOMENTS
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POINT   1           X           Y           Z (BOHR)    CHARGE
-1.311953   -0.518842   -0.178718        0.00 (A.U.)
DX          DY          DZ         /D/  (DEBYE)
0.507662    1.267141   -0.880123    1.624187
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =     3.27 TOTAL CPU TIME =    24280.0 (  404.7 MIN)
TOTAL WALL CLOCK TIME=    64525.7 SECONDS, CPU UTILIZATION IS  37.63%
$VIB
IVIB=   0 IATOM=   0 ICOORD=   0 E=     -425.4260567991
1.940115696E-05 1.111804117E-05-5.011649907E-05 3.011129598E-05-6.244324761E-05
1.223324882E-05-1.789015807E-06-5.984804459E-05 7.609807939E-06-4.964542034E-05
2.908242298E-05 7.004956313E-05 4.598353000E-05-6.461821319E-06-8.020350830E-05
-1.030400090E-05-8.546892445E-06 1.589771070E-05 1.813880817E-05-7.351906735E-05
-2.764251443E-05 3.052892233E-05 6.069220895E-05-1.819141611E-05-2.729061619E-06
3.840975329E-05-2.297464509E-05-3.495630611E-05-1.122411270E-05-1.093017553E-05
2.236970871E-05-1.879848892E-06 9.775695119E-06-5.903328428E-06-3.103181007E-06
1.450080206E-05-1.659420551E-05 4.200703573E-05 2.341021214E-05-1.835362806E-05
2.089028979E-05 3.258957694E-05-5.714678131E-05-4.153799506E-06-1.556961753E-06
2.517381844E-07-4.174781130E-06 9.041455898E-06 2.880289874E-05 3.168420134E-05
-1.279726382E-05-2.023948519E-06-7.649098152E-06-6.938060459E-06 2.284057315E-05
-2.966145821E-05 7.384710365E-06-5.831538657E-06 1.768272494E-05 1.148808493E-05
-8.359951914E-06-1.700488697E-06-3.607023960E-08-5.343931596E-06 2.507598394E-05
2.108887945E-06 5.524865372E-07-2.276820523E-06 1.529735881E-05
5.076616999E-01 1.267140863E+00-8.801225312E-01
......END OF GEOMETRY SEARCH......
STEP CPU TIME =     0.20 TOTAL CPU TIME =    24280.2 (  404.7 MIN)
TOTAL WALL CLOCK TIME=    64525.9 SECONDS, CPU UTILIZATION IS  37.63%
1324465  WORDS OF DYNAMIC MEMORY USED
EXECUTION OF GAMESS TERMINATED NORMALLY Thu Mar  1 07:29:06 2007
DDI: 262808 bytes (0.3 MB / 0 MWords) used by master data server.
```

Trans 4,4-dimethylpentanoate

```
ECHO OF THE FIRST FEW INPUT CARDS -
INPUT CARD> $CONTRL RUNTYP=OPTIMIZE $END
INPUT CARD> $DFT DFTTYP=B3LYP $END
INPUT CARD> $BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.T. $END
INPUT CARD> $CONTRL ICHARG=-1 $END
INPUT CARD> $SYSTEM BALTYP=LOOP $END
INPUT CARD> $CONTRL MAXIT=30 $END
INPUT CARD> $SYSTEM TIMLIM=1200 MWORDS=62.50 $END
INPUT CARD>
INPUT CARD> $DATA
INPUT CARD>untitled
INPUT CARD>C1
INPUT CARD> C           6.0  -0.4649796451  -0.3360827210   0.4710339737
INPUT CARD> C           6.0  -1.4736445272  -0.1085976129  -0.6614266386
INPUT CARD> C           6.0  -2.7479301682  -1.0275110361  -0.5714862483
INPUT CARD> C           6.0   0.9615054808   0.2557835882   0.3045295967
INPUT CARD> C           6.0   0.9195573641   1.7916945109   0.1602364830
INPUT CARD> C           6.0   1.6678103538  -0.3535159848  -0.9238897915
INPUT CARD> C           6.0   1.7911652358  -0.1021776977   1.5564842094
INPUT CARD> O           8.0  -2.5662275998  -2.1829091177  -0.0955840147
INPUT CARD> O           8.0  -3.8097869242  -0.5189087373  -1.0237881079
INPUT CARD> H           1.0  -0.3915389622  -1.4214603833   0.6187405975
INPUT CARD> H           1.0  -0.8922107022   0.0626271799   1.4051379722
INPUT CARD> H           1.0  -1.0098213429  -0.3334057891  -1.6332718158
INPUT CARD> H           1.0  -1.8080686951   0.9349520207  -0.7069937235
INPUT CARD> H           1.0   0.4770861646   2.2559719952   1.0512917297
INPUT CARD> H           1.0   0.3180902063   2.0907714467  -0.7044080523
INPUT CARD> H           1.0   1.9318171212   2.2004995735   0.0319657719
INPUT CARD> H           1.0   2.7113168598  -0.0143314908  -0.9873433629
INPUT CARD> H           1.0   1.1726742514  -0.0793011318  -1.8618744862
INPUT CARD> H           1.0   1.6708585840  -1.4491915153  -0.8630733318
INPUT CARD> H           1.0   2.8131952673   0.2964567406   1.4859082402
INPUT CARD> H           1.0   1.8599115294  -1.1907539212   1.6776295374
INPUT CARD> H           1.0   1.3327381484   0.3030200834   2.4682614618
INPUT CARD> $END
62000000 WORDS OF MEMORY AVAILABLE


NSERCH= 14     ENERGY=    -424.8667461

-----------------------
GRADIENT (HARTREE/BOHR)
-----------------------
ATOM            ZNUC       DE/DX         DE/DY         DE/DZ
------------------------------------------------------------
1  C            6.0    -0.0000071     0.0000079     0.0000276
2  C            6.0     0.0000358     0.0000593    -0.0000413
3  C            6.0     0.0000079     0.0000012     0.0000304
4  C            6.0    -0.0000041    -0.0000241    -0.0000388
5  C            6.0    -0.0000328    -0.0000218    -0.0000116
6  C            6.0    -0.0000051    -0.0000368     0.0000300
7  C            6.0    -0.0000153    -0.0000033    -0.0000059
8  O            8.0    -0.0000062    -0.0000542     0.0000047
9  O            8.0    -0.0000071     0.0000070    -0.0000187
10  H           1.0     0.0000187     0.0000072     0.0000010
11  H           1.0     0.0000049    -0.0000126     0.0000011
12  H           1.0     0.0000000    -0.0000058     0.0000026
13  H           1.0     0.0000068     0.0000081     0.0000071
14  H           1.0     0.0000144     0.0000151     0.0000049
15  H           1.0     0.0000082    -0.0000035     0.0000031
16  H           1.0     0.0000000     0.0000090     0.0000067
17  H           1.0     0.0000038     0.0000162    -0.0000167
18  H           1.0    -0.0000051     0.0000159     0.0000039
19  H           1.0    -0.0000188     0.0000118     0.0000064
20  H           1.0     0.0000008    -0.0000010     0.0000055
21  H           1.0    -0.0000020     0.0000027    -0.0000027
22  H           1.0     0.0000025     0.0000017     0.0000005
```

MAXIMUM GRADIENT = 0.0000593 RMS GRADIENT = 0.0000179

***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.4661155399	-0.3389669151	0.4630718616
C	6.0	-1.4786999292	-0.0910457249	-0.6632015911
C	6.0	-2.7398814092	-1.0252708321	-0.5725300895
C	6.0	0.9613785660	0.2528062168	0.3027966492
C	6.0	0.9193619840	1.7867667578	0.1391611643
C	6.0	1.6788478444	-0.3713251318	-0.9120821655
C	6.0	1.7775006325	-0.0889134348	1.5682442637
O	8.0	-2.5028608518	-2.2350732209	-0.2998700851
O	8.0	-3.8476047926	-0.4736364222	-0.8133003913
H	1.0	-0.3910991133	-1.4270119935	0.5888289736
H	1.0	-0.8900202751	0.0459359523	1.4048191070
H	1.0	-1.0130948070	-0.3003355564	-1.6370299048
H	1.0	-1.8169927047	0.9518568585	-0.6814561889
H	1.0	0.4676854900	2.2623257514	1.0193611524
H	1.0	0.3259690912	2.0741905241	-0.7350704216
H	1.0	1.9324290441	2.1945712042	0.0151053751
H	1.0	2.7194628875	-0.0235288452	-0.9774827498
H	1.0	1.1845818719	-0.1170842228	-1.8561129898
H	1.0	1.6907604622	-1.4654717307	-0.8323817983
H	1.0	2.8028739938	0.3014216799	1.5015180957
H	1.0	1.8373193503	-1.1755318400	1.7090912206
H	1.0	1.3117162050	0.3369509255	2.4666005126

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1 C	6.274527	-0.274527	6.335478	-0.335478
2 C	6.348563	-0.348563	6.334973	-0.334973
3 C	5.702321	0.297679	5.848956	0.151044
4 C	5.529625	0.470375	6.240879	-0.240879
5 C	6.551901	-0.551901	6.466318	-0.466318
6 C	6.606049	-0.606049	6.459140	-0.459140
7 C	6.485378	-0.485378	6.466247	-0.466247
8 O	8.611129	-0.611129	8.553252	-0.553252
9 O	8.629766	-0.629766	8.546684	-0.546684
10 H	0.824730	0.175270	0.801150	0.198850
11 H	0.885864	0.114136	0.823762	0.176238
12 H	0.888012	0.111988	0.825313	0.174687
13 H	0.869238	0.130762	0.828453	0.171547
14 H	0.867573	0.132427	0.826518	0.173482
15 H	0.846207	0.153793	0.818904	0.181096
16 H	0.882411	0.117589	0.838741	0.161259
17 H	0.883011	0.116989	0.839856	0.160144
18 H	0.855312	0.144688	0.823797	0.176203
19 H	0.854319	0.145681	0.824468	0.175532
20 H	0.879870	0.120130	0.839298	0.160702
21 H	0.858430	0.141570	0.828619	0.171381
22 H	0.865765	0.134235	0.829193	0.170807

BOND ORDER AND VALENCE ANALYSIS BOND ORDER THRESHOLD=0.050

ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER
1	2	1.535	0.972	1	3	2.591	-0.061	1	4	1.554	0.978
1	7	2.514	-0.094	1	8	2.885	0.214	1	10	1.098	0.912
1	11	1.102	0.944	1	12	2.171	-0.052	2	3	1.572	1.020
2	8	2.404	-0.233	2	12	1.100	0.946	2	13	1.097	0.955
3	8	1.263	1.646	3	9	1.261	1.638	3	13	2.185	0.058
4	5	1.543	0.772	4	6	1.543	0.766	4	7	1.544	0.638
4	8	4.307	-0.131	4	15	2.191	-0.059	4	20	2.198	-0.060
4	21	2.187	-0.104	4	22	2.194	-0.092	5	14	1.098	1.011
5	15	1.095	1.028	5	16	1.099	1.004	6	8	4.619	0.057

```
6     17  1.099  1.007        6  18  1.096  1.011        6  19  1.097  1.007
7     20  1.099  1.019        7  21  1.097  1.043        7  22  1.098  1.037

                    TOTAL       BONDED        FREE
ATOM               VALENCE     VALENCE     VALENCE
1 C                 3.754       3.754       0.000
2 C                 3.546       3.546       0.000
3 C                 4.384       4.384       0.000
4 C                 2.497       2.497       0.000
5 C                 3.691       3.691       0.000
6 C                 3.833       3.833       0.000
7 C                 3.447       3.447       0.000
8 O                 1.524       1.524       0.000
9 O                 1.535       1.535       0.000
10 H                0.941       0.941       0.000
11 H                0.945       0.945       0.000
12 H                0.946       0.946       0.000
13 H                0.945       0.945       0.000
14 H                0.948       0.948       0.000
15 H                0.944       0.944       0.000
16 H                0.948       0.948       0.000
17 H                0.948       0.948       0.000
18 H                0.948       0.948       0.000
19 H                0.945       0.945       0.000
20 H                0.948       0.948       0.000
21 H                0.946       0.946       0.000
22 H                0.948       0.948       0.000

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ELECTROSTATIC MOMENTS
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POINT   1           X           Y           Z (BOHR)    CHARGE
-1.222405   -0.558465   -0.174174       -1.00 (A.U.)
DX          DY          DZ          /D/  (DEBYE)
10.784183    4.550776    1.794988   11.841881
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =     3.13 TOTAL CPU TIME =    19929.0 (  332.2 MIN)
TOTAL WALL CLOCK TIME=    46745.8 SECONDS, CPU UTILIZATION IS  42.63%
$VIB
IVIB=   0 IATOM=   0 ICOORD=   0 E=     -424.8667461222
-7.129463989E-06 7.875220860E-06 2.760449333E-05 3.580796767E-05 5.929440518E-05
-4.132583759E-05 7.885752296E-06 1.179121053E-06 3.043242042E-05-4.129862629E-06
-2.409951573E-05-3.884364686E-05-3.284553473E-05-2.179278578E-05-1.156594439E-05
-5.067256355E-06-3.680456212E-05 2.999320527E-05-1.534748297E-05-3.260982221E-06
-5.853766082E-06-6.244271489E-06-5.415549447E-05 4.678910030E-06-7.127630110E-06
7.045479386E-06-1.874870039E-05 1.872611334E-05 7.166414424E-06 9.865237872E-07
4.878631006E-06-1.261805617E-05 1.148249183E-06-1.457359858E-08-5.795764034E-06
2.640348564E-06 6.844965415E-06 8.087057619E-06 7.087034483E-06 1.436070629E-05
1.511883398E-05 4.894303204E-06 8.207962092E-06-3.474429498E-06 3.135306531E-06
1.948354427E-08 8.955811354E-06 6.743340335E-06 3.784677063E-06 1.616452495E-05
-1.665314830E-05-5.081451310E-06 1.590382283E-05 3.879218788E-06-1.879371651E-05
1.181641834E-05 6.411544046E-06 7.716326416E-07-1.041158835E-06 5.490875917E-06
-2.038482352E-06 2.727403616E-06-2.668046865E-06 2.531834668E-06 1.708235263E-06
5.333166008E-07
1.078418328E+01 4.550775649E+00 1.794987899E+00
......END OF GEOMETRY SEARCH......
STEP CPU TIME =     0.19 TOTAL CPU TIME =    19929.2 (  332.2 MIN)
TOTAL WALL CLOCK TIME=    46746.0 SECONDS, CPU UTILIZATION IS  42.63%
1309083  WORDS OF DYNAMIC MEMORY USED
EXECUTION OF GAMESS TERMINATED NORMALLY Sun Apr  1 04:06:28 2007
DDI: 262808 bytes (0.3 MB / 0 MWords) used by master data server.
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Altona Equations

3-(Trimethylsilyl)-propionic acid

J_{13} = 6.0411 Hz × (Fraction Gauche) + 3.8713 Hz
J_{14} = -12.1109 Hz × (Fraction Gauche) + 15.9726 Hz

3-(Trimethylsilyl)-propionate

H_2O
J_{13} = 6.25272 Hz × (Fraction Gauche) + 3.85247 Hz
J_{14} = -12.3546 Hz × (Fraction Gauche) + 16.2574 Hz

Ethanol, Methanol, *iso*-Propanol
J_{13} = 6.22651 Hz × (Fraction Gauche) + 3.85364 Hz
J_{14} = -12.3213 Hz × (Fraction Gauche) + 16.2189 Hz

tert-Butanol
J_{13} = 6.27828 Hz × (Fraction Gauche) + 3.85173 Hz
J_{14} = -12.3882 Hz × (Fraction Gauche) + 16.296 Hz

DMSO, THF, Toluene
J_{13} = 6.10083 Hz × (Fraction Gauche) + 3.86408 Hz
J_{14} = -12.1744 Hz × (Fraction Gauche) + 16.0476 Hz

4,4-dimethylpentanoic acid

J_{13} = 4.98418 Hz × (Fraction Gauche) + 3.88316 Hz
J_{14} = -10.695 Hz × (Fraction Gauche) + 14.3363 Hz

4,4-dimethylpentanoate

J_{13} = 5.12908 Hz × (Fraction Gauche) + 3.86806 Hz
J_{14} = -10.8564 Hz × (Fraction Gauche) + 14.525 Hz